Nitroethane

79-24-3 | DTXSID8020969

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 117 °C

Global applicability domain: Inside

Local applicability domain index: 6.59e-01

Confidence level: 7.33e-01

Nearest Neighbors from the Training Set

Image not found
Nitroethane
Measured: 114
Predicted: 117

Image not found
Chloronitromethane
Measured: 123
Predicted: 120

Image not found
Acetoxime
Measured: 136
Predicted: 128

Image not found
Ethene, nitro-
Measured: 98.5
Predicted: 108